Phthalic acid, 5-bromo-2-methoxybenzyl butyl ester

Inchi: InChI=1S/C20H21BrO5/c1-3-4-11-25-19(22)16-7-5-6-8-17(16)20(23)26-13-14-12-15(21)

InchiKey: KZJIFANCWXWHBU-UHFFFAOYSA-N

Formula: C20H21BrO5

SMILES: CCCCOC(=O)c1ccccc1C(=O)OCc1cc(Br)ccc1OC

Mol. weight [g/mol]: 421.28

Physical Properties

Property code	Value	Unit	Source
gf	-245.07	kJ/mol	Joback Method
hf	-612.97	kJ/mol	Joback Method
hfus	46.52	kJ/mol	Joback Method
hvap	93.81	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	4.772		Crippen Method
mcvol	283.390	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	2799.00		NIST Webbook
rinpol	2799.00		NIST Webbook
tb	966.46	K	Joback Method
tc	1201.04	K	Joback Method
tf	631.91	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.96	J/mol×K	966.46	Joback Method
cpg	849.08	J/mol×K	1005.56	Joback Method
cpg	858.78	J/mol×K	1044.65	Joback Method
cpg	867.10	J/mol×K	1083.75	Joback Method
cpg	874.04	J/mol×K	1122.85	Joback Method
cpg	879.63	J/mol×K	1161.95	Joback Method
cpg	883.89	J/mol×K	1201.04	Joback Method
dvisc	0.0002036	Pa×s	631.91	Joback Method

dvisc	0.0001342	Pa×s	687.67	Joback Method
dvisc	0.0000941	Pa×s	743.43	Joback Method
dvisc	0.0000694	Pa×s	799.19	Joback Method
dvisc	0.0000532	Pa×s	854.94	Joback Method
dvisc	0.0000422	Pa×s	910.70	Joback Method
dvisc	0.0000343	Pa×s	966.46	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382866&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume